Full wwPDB EM Validation Report ⓘ

Jul 15, 2024 – 12:29 PM JST

PDB ID	:	8XYZ
EMDB ID	:	EMD-38784
Title	:	The structure of fox ACE2 and PT RBD complex
Authors	:	sun, J.Q.
Deposited on	:	2024-01-20
Resolution	:	2.96 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

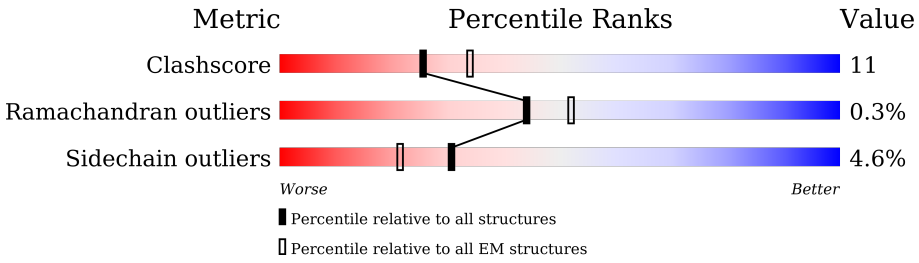
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	B	273	46% 25% . 29%
2	A	613	77% 20% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6429 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Signal peptide, Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	195	Total	C	N	O	S	0	0
			1543	989	257	289	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	542	HIS	-	expression tag	UNP P0DTC2
B	543	HIS	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	596	Total	C	N	O	S	0	0
			4885	3123	810	923	29		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

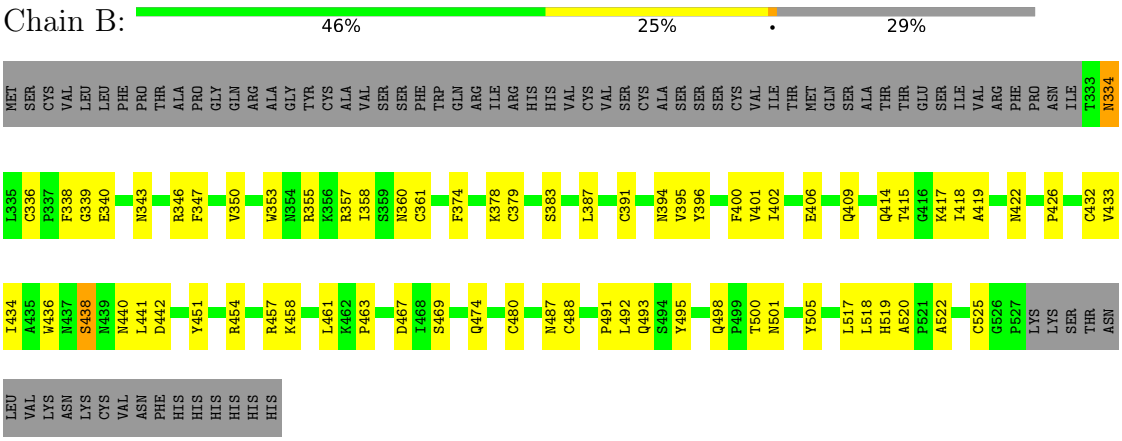
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

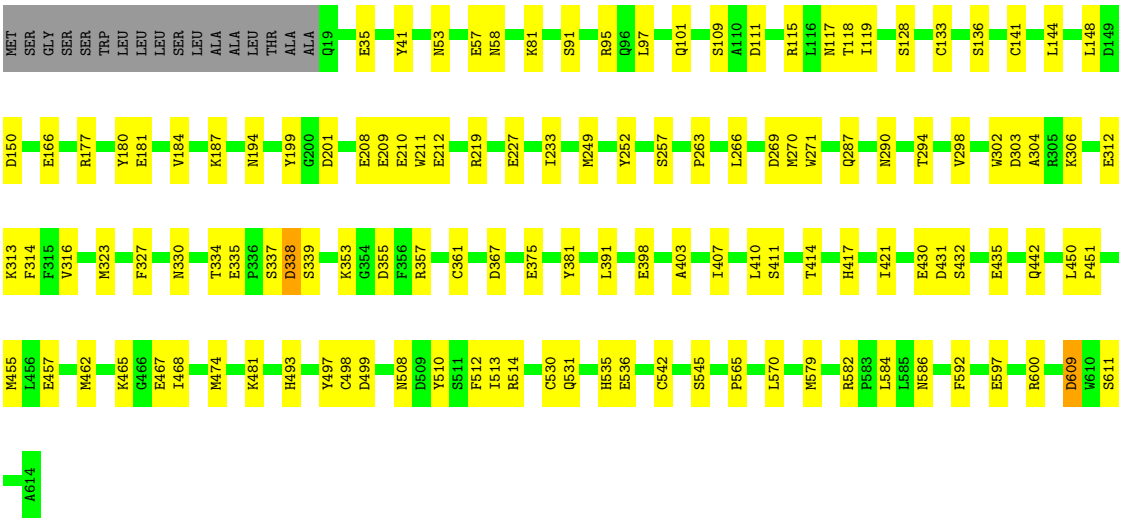
- Molecule 1: Signal peptide, Spike protein S1

Chain B:



- Molecule 2: Angiotensin-converting enzyme

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217439	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	B	0.32	0/1587	0.67	0/2161
2	A	0.36	0/5027	0.55	0/6830
All	All	0.35	0/6614	0.58	0/8991

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1543	0	1468	69	0
2	A	4885	0	4654	75	0
3	A	1	0	0	0	0
All	All	6429	0	6122	141	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (141) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:LEU:HD12	1:B:517:LEU:O	1.59	1.02
1:B:379:CYS:SG	1:B:433:VAL:N	2.52	0.82
2:A:303:ASP:OD1	2:A:304:ALA:N	2.15	0.79
2:A:133:CYS:HB3	2:A:141:CYS:SG	2.27	0.74
1:B:358:ILE:HD12	1:B:395:VAL:HG12	1.71	0.73
1:B:374:PHE:CE2	1:B:434:ILE:CG2	2.73	0.72
1:B:336:CYS:SG	1:B:338:PHE:CD1	2.79	0.72
1:B:336:CYS:HB2	1:B:361:CYS:SG	2.30	0.72
1:B:336:CYS:SG	1:B:338:PHE:HD1	2.16	0.69
1:B:518:LEU:HD23	1:B:519:HIS:O	1.94	0.68
1:B:350:VAL:HG11	1:B:402:ILE:CG2	2.24	0.67
1:B:374:PHE:CE1	1:B:436:TRP:HB3	2.30	0.66
2:A:177:ARG:HB2	2:A:498:CYS:HB2	1.77	0.66
1:B:336:CYS:HG	1:B:338:PHE:HD1	1.32	0.66
2:A:530:CYS:HG	2:A:542:CYS:HG	0.65	0.65
1:B:334:ASN:ND2	1:B:360:ASN:O	2.29	0.64
2:A:41:TYR:HD2	2:A:353:LYS:HE2	1.64	0.63
1:B:454:ARG:NH2	1:B:469:SER:O	2.32	0.63
1:B:457:ARG:HH22	1:B:467:ASP:HB3	1.64	0.63
2:A:355:ASP:OD2	2:A:357:ARG:NH1	2.32	0.63
1:B:374:PHE:CE2	1:B:434:ILE:HG23	2.35	0.62
1:B:374:PHE:CD2	1:B:434:ILE:HG23	2.35	0.62
2:A:111:ASP:OD2	2:A:111:ASP:N	2.32	0.62
1:B:391:CYS:HB3	1:B:525:CYS:SG	2.40	0.61
2:A:41:TYR:CD2	2:A:353:LYS:HE2	2.36	0.61
2:A:474:MET:CE	2:A:499:ASP:H	2.14	0.61
1:B:426:PRO:HD3	1:B:463:PRO:HB3	1.82	0.60
2:A:91:SER:O	2:A:95:ARG:HG2	2.01	0.60
1:B:374:PHE:HE2	1:B:434:ILE:HG21	1.66	0.60
1:B:378:LYS:O	1:B:378:LYS:HG3	2.01	0.60
1:B:357:ARG:HG3	1:B:396:TYR:HE1	1.67	0.60
2:A:194:ASN:O	2:A:194:ASN:OD1	2.20	0.59
2:A:403:ALA:O	2:A:407:ILE:HG13	2.02	0.59
2:A:53:ASN:O	2:A:58:ASN:ND2	2.37	0.58
2:A:233:ILE:HD11	2:A:584:LEU:HD22	1.85	0.58
2:A:263:PRO:HB2	2:A:266:LEU:HD13	1.86	0.58
1:B:374:PHE:HE2	1:B:434:ILE:CG2	2.17	0.57
1:B:350:VAL:HG12	1:B:400:PHE:CD1	2.40	0.57
1:B:409:GLN:NE2	1:B:419:ALA:H	2.02	0.57
2:A:609:ASP:OD2	2:A:609:ASP:N	2.37	0.56
2:A:530:CYS:CB	2:A:542:CYS:HG	2.16	0.56
1:B:357:ARG:HG3	1:B:396:TYR:CE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:201:ASP:OD1	2:A:219:ARG:NH1	2.39	0.56
2:A:530:CYS:SG	2:A:535:HIS:HB3	2.45	0.56
1:B:518:LEU:HD22	1:B:520:ALA:HB2	1.88	0.55
2:A:115:ARG:O	2:A:118:THR:HG22	2.07	0.55
2:A:109:SER:OG	2:A:111:ASP:OD2	2.23	0.54
1:B:379:CYS:SG	1:B:433:VAL:HG12	2.48	0.54
2:A:81:LYS:HA	2:A:101:GLN:HE21	1.73	0.54
2:A:115:ARG:O	2:A:119:ILE:HD13	2.08	0.54
2:A:335:GLU:HB2	2:A:361:CYS:HB3	1.89	0.53
2:A:462:MET:HB3	2:A:468:ILE:HG13	1.89	0.53
1:B:353:TRP:CH2	1:B:355:ARG:NH2	2.77	0.53
1:B:440:ASN:OD1	1:B:441:LEU:HD22	2.09	0.53
1:B:401:VAL:HG11	1:B:451:TYR:CE1	2.43	0.53
1:B:379:CYS:SG	1:B:432:CYS:HA	2.50	0.52
1:B:353:TRP:HH2	1:B:355:ARG:NH2	2.08	0.52
2:A:208:GLU:OE2	2:A:219:ARG:NE	2.38	0.52
1:B:501:ASN:N	1:B:501:ASN:HD22	2.08	0.51
2:A:312:GLU:O	2:A:316:VAL:HG12	2.10	0.51
2:A:455:MET:SD	2:A:481:LYS:HG2	2.50	0.51
1:B:394:ASN:N	1:B:394:ASN:OD1	2.42	0.51
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.75	0.51
1:B:498:GLN:HB2	1:B:501:ASN:HD21	1.75	0.51
1:B:493:GLN:NE2	2:A:35:GLU:OE1	2.43	0.50
1:B:358:ILE:HD12	1:B:395:VAL:CG1	2.40	0.50
1:B:438:SER:OG	1:B:442:ASP:OD2	2.29	0.49
2:A:465:LYS:HD2	2:A:467:GLU:HG3	1.92	0.49
1:B:409:GLN:HE21	1:B:419:ALA:H	1.59	0.49
2:A:430:GLU:HB2	2:A:435:GLU:OE2	2.12	0.49
1:B:336:CYS:SG	1:B:338:PHE:CE1	2.99	0.49
2:A:410:LEU:HD11	2:A:442:GLN:HE22	1.78	0.48
2:A:474:MET:HE3	2:A:499:ASP:H	1.78	0.48
1:B:518:LEU:HD23	1:B:519:HIS:C	2.34	0.48
2:A:431:ASP:OD2	2:A:432:SER:N	2.47	0.48
1:B:374:PHE:CE1	1:B:436:TRP:CB	2.97	0.47
2:A:493:HIS:CG	2:A:497:TYR:HD2	2.32	0.47
2:A:530:CYS:CB	2:A:542:CYS:SG	3.02	0.47
2:A:180:TYR:O	2:A:184:VAL:HG12	2.14	0.47
2:A:294:THR:O	2:A:298:VAL:HG23	2.14	0.47
1:B:438:SER:OG	1:B:438:SER:O	2.32	0.46
2:A:187:LYS:HD2	2:A:199:TYR:CZ	2.49	0.46
2:A:270:MET:HA	2:A:270:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:CYS:CB	1:B:525:CYS:SG	3.03	0.46
1:B:350:VAL:HG11	1:B:402:ILE:HG22	1.96	0.46
2:A:323:MET:HE2	2:A:327:PHE:CD1	2.50	0.46
1:B:379:CYS:SG	1:B:432:CYS:HB3	2.56	0.46
2:A:209:GLU:OE2	2:A:565:PRO:HG3	2.16	0.46
1:B:474:GLN:HB2	1:B:480:CYS:SG	2.56	0.45
1:B:402:ILE:HD12	1:B:406:GLU:HB2	1.98	0.45
2:A:474:MET:HE1	2:A:499:ASP:H	1.79	0.45
2:A:287:GLN:HA	2:A:287:GLN:OE1	2.17	0.45
1:B:498:GLN:HB2	1:B:501:ASN:ND2	2.32	0.45
1:B:379:CYS:SG	1:B:432:CYS:CA	3.04	0.45
2:A:530:CYS:HB2	2:A:542:CYS:SG	2.57	0.44
1:B:391:CYS:SG	1:B:522:ALA:HB3	2.58	0.44
2:A:536:GLU:N	2:A:536:GLU:OE2	2.51	0.44
1:B:480:CYS:CB	1:B:488:CYS:SG	3.05	0.44
2:A:252:TYR:CE2	2:A:266:LEU:HD23	2.53	0.44
1:B:457:ARG:CZ	1:B:461:LEU:HD21	2.47	0.43
2:A:330:ASN:HB3	2:A:357:ARG:NH2	2.33	0.43
2:A:411:SER:O	2:A:414:THR:HG22	2.17	0.43
2:A:450:LEU:HB2	2:A:451:PRO:HD3	1.99	0.43
1:B:409:GLN:HE22	1:B:418:ILE:H	1.66	0.43
2:A:302:TRP:NE1	2:A:306:LYS:NZ	2.61	0.43
2:A:97:LEU:HD12	2:A:97:LEU:HA	1.88	0.43
1:B:418:ILE:HA	1:B:422:ASN:ND2	2.33	0.43
1:B:458:LYS:HA	1:B:458:LYS:HE2	2.00	0.43
1:B:500:THR:OG1	2:A:41:TYR:OH	2.36	0.43
2:A:181:GLU:OE2	2:A:181:GLU:HA	2.19	0.43
2:A:367:ASP:OD2	2:A:367:ASP:N	2.51	0.43
1:B:353:TRP:HH2	1:B:355:ARG:HH21	1.66	0.43
1:B:505:TYR:CD2	2:A:353:LYS:HG2	2.54	0.43
2:A:457:GLU:HG2	2:A:513:ILE:HD13	2.00	0.43
1:B:491:PRO:HG2	1:B:492:LEU:HD12	2.01	0.43
2:A:211:TRP:CD1	2:A:212:GLU:HG3	2.54	0.42
2:A:313:LYS:HE3	2:A:313:LYS:HB2	1.77	0.42
1:B:480:CYS:CB	1:B:488:CYS:HG	2.25	0.42
2:A:144:LEU:HA	2:A:148:LEU:HB2	2.00	0.42
2:A:597:GLU:OE1	2:A:600:ARG:NH2	2.51	0.42
1:B:346:ARG:NH1	1:B:347:PHE:O	2.52	0.42
1:B:339:GLY:O	1:B:343:ASN:ND2	2.53	0.42
1:B:336:CYS:CB	1:B:361:CYS:SG	3.05	0.42
2:A:375:GLU:HA	2:A:375:GLU:OE2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:SER:H	1:B:387:LEU:HD22	1.85	0.41
1:B:518:LEU:HD23	1:B:519:HIS:N	2.35	0.41
2:A:57:GLU:H	2:A:57:GLU:CD	2.23	0.41
2:A:133:CYS:CB	2:A:141:CYS:SG	3.03	0.41
2:A:430:GLU:H	2:A:430:GLU:HG2	1.53	0.41
1:B:517:LEU:O	1:B:517:LEU:CD1	2.47	0.41
2:A:410:LEU:HD12	2:A:410:LEU:HA	1.91	0.41
2:A:432:SER:HA	2:A:435:GLU:HG2	2.01	0.41
2:A:290:ASN:OD1	2:A:290:ASN:N	2.54	0.41
2:A:579:MET:H	2:A:579:MET:HG3	1.67	0.41
1:B:374:PHE:CD1	1:B:436:TRP:HB3	2.55	0.41
2:A:227:GLU:OE2	2:A:227:GLU:HA	2.21	0.41
2:A:391:LEU:HD23	2:A:391:LEU:HA	1.85	0.41
2:A:398:GLU:OE1	2:A:514:ARG:NH2	2.54	0.40
2:A:570:LEU:HD12	2:A:570:LEU:HA	1.82	0.40
2:A:209:GLU:HG3	2:A:210:GLU:N	2.35	0.40
2:A:417:HIS:O	2:A:421:ILE:HG12	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	193/273 (71%)	187 (97%)	6 (3%)	0	100	100
2	A	594/613 (97%)	583 (98%)	9 (2%)	2 (0%)	41	73
All	All	787/886 (89%)	770 (98%)	15 (2%)	2 (0%)	44	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	337	SER

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Mol	Chain	Res	Type
2	A	338	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	168/239 (70%)	160 (95%)	8 (5%)	25 59
2	A	530/542 (98%)	506 (96%)	24 (4%)	27 61
All	All	698/781 (89%)	666 (95%)	32 (5%)	31 60

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	334	ASN
1	B	340	GLU
1	B	414	GLN
1	B	415	THR
1	B	417	LYS
1	B	438	SER
1	B	487	ASN
1	B	495	TYR
2	A	117	ASN
2	A	128	SER
2	A	136	SER
2	A	150	ASP
2	A	166	GLU
2	A	249	MET
2	A	257	SER
2	A	269	ASP
2	A	271	TRP
2	A	314	PHE
2	A	334	THR
2	A	338	ASP
2	A	339	SER
2	A	381	TYR

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Mol	Chain	Res	Type
2	A	508	ASN
2	A	510	TYR
2	A	512	PHE
2	A	531	GLN
2	A	545	SER
2	A	582	ARG
2	A	586	ASN
2	A	592	PHE
2	A	609	ASP
2	A	611	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	354	ASN
1	B	409	GLN
1	B	414	GLN
1	B	501	ASN
2	A	60	GLN
2	A	96	GLN
2	A	101	GLN
2	A	117	ASN
2	A	134	ASN
2	A	300	GLN
2	A	442	GLN
2	A	508	ASN
2	A	535	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.